Framework for a chemical substance reporting system.

Framework for a Chemical Substance Reporting System

Sukhraj Singh Takhar
Subject Matter Expert – Materials Management and Chemical Reporting, Assent Compliance Inc. & PhD Research Student, College of Engineering and Technology, University of Derby,
Derby, DE22 3AW, United Kingdom
e-mail: Raj.Takhar@assentcompliance.com

Kapila Liyanage
Senior Lecturer, College of Engineering and Technology, University of Derby
Derby, DE22 3AW United Kingdom.
e-mail: K.Liyanage@derby.ac.uk

***Abstract*—Chemical regulations exist to control hazardous chemical substance use within society. As more chemical substances become more regulated, industry must adapt and develop mechanisms to analyze and report data on substances used on their own, in mixtures or within materials. A chemical substance reporting system is required to ensure compliance by identifying the chemical substances used within a product, which can then be compared against regulated chemical substance lists to identify potential business risks, as well as providing safety data to consumers. This paper contributes to material compliance reporting literature by identifying a research gap and presenting a framework model to enable chemical substance information to be collated (internal and external) to allow for accurate chemical substance reporting.**

Keywords-material compliance reporting; supply chain management; material declaration; transformation cycle; chemical regulation

I. INTRODUCTION

Regulations exist to impose a consistent set of norm/behaviours upon society. Chemical regulations first appeared in the 1960's (European Commission, 1967) as the Thalidomide and Asbestos scandals raised public awareness on the effects of hazardous chemicals. Chemical regulations look to ensure chemical substance usage is identified, tracked and where applicable controlled or restricted (Regulation of Chemicals wiki, 2017). The evolution of chemical regulations such as the European Union (EU) Restriction of Hazardous Substances (RoHS) (European Commission, 2002; European Commission, 2011); EU Registration Evaluation Authorisation and restriction of CHemicals (REACH) (European Commission, 2006) and other international regulations has facilitated the need to record and manage increasingly large amounts of chemical substance related information (Selin, 2011; Molander and Rudén, 2012; Sivaprakash, Karthikeyan, Joseph, 2014). Chemical regulations exist to control and limit the use of hazardous chemicals; to protect the welfare of humans; the environmental and therefore society.

The traditional focus of engineering organizations (Skinner, 1978) departmentalizes data within functional areas using the data, thereby creating data silos, making chemical substance reporting difficult to implement.

The purpose of this paper is to examine the information paradox which has arisen and present a framework which will enable an organization to implement a base layer chemical substance reporting system.

II. METHODOLOGY

A three-step methodology approach was used based on (1) initial literature review of chemical regulations, automotive and electronic industry implementation approaches, business strategies, and data modelling; (2) previous experiences from working as a system design engineer within Engineering, IT and Aerospace and Defence (AD) industries, including drafting the initial IPC-1754 material data exchange standard for AD and Heavy Machinery (HM) industries; (3) expert interviews with AD companies.

III. FINDINGS

A. *Supply Chain Evolution*

The term 'Article Transformation Cycle' describes the process of taking raw materials, processing substances and mixtures to produce finished articles. (Fig. 1) depicts the article transformation cycle.

A supply chain can be considered a collection of organizations / elements, selling / flowing articles and services, downstream and upstream across a supply chain. The traditional supply chain paradox focused on (1) maintaining quality deliverables; (2) reducing supply chain costs to maximize profit; (3) increasing customer satisfaction levels (Dias and Ierapetritou, 2017; Porter, 1980). Supply chains have evolved from producing simple but labour intensive articles to modern day highly complex modern articles which consist of globally accessible chemical substances, material and materials (Woinaroschy, 2016).

B. *Impacts of Chemical Regulation Changes*

Each new piece of chemical regulation presents industry with potentially new supply chain risk(s) (Fig. 2).

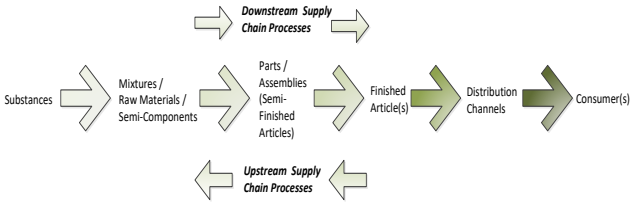

Figure 1. Article transformation cycle (simple supply chain)

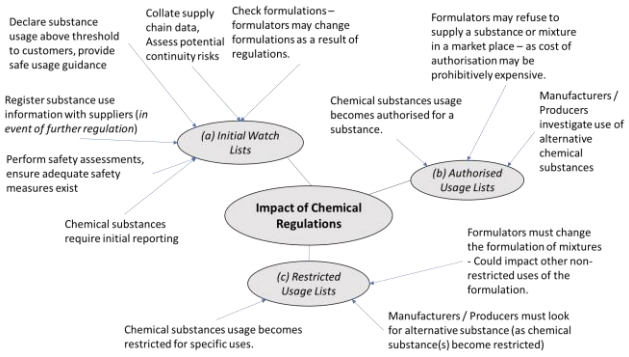

Figure 2. Impact of chemical regulations

Chemical regulations define lists of substances against which specific actions need to be undertaken, such as (1) notifications to regulators; (2) material declarations from the supply chain; (3) declarations to consumers; (4) safe use guidance, (5) request authorized use of a substance request; (6) even prohibited use of a substance, this information requires substance identification at the article level (Ashby, 2009; Molander et al, 2012) Early research found compared reporting requirements varied between regulations (Molander and Rudén, 2012).

C. Multiple Declarable Substance Lists

Increasing numbers of chemical regulations have resulted in multiple lists of substances (ECHA candidate list, 2017; ECHA authorisations list, 2017; ECHA restrictions list, 2017) having to being constantly monitored. Industry had to develop harmonized substance lists which first appeared from the mid 2000's notably in the Automotive (IMDS, 2017), Electronics (IPC, 2017; IEC, 2017) and AD sectors (IAEG, 2017).

D. The Information Paradox – Traditional Internal Data Supply Chain Information Flows

Chemical substance reporting systems require connected design, engineering, supply chain, distribution systems which can handle data consistently being received / transmitted. A data supply chain is the information flow (internal or external), which requires clear and concise data flow analysis, which can then be readily absorbed by sub-systems, against which appropriate risk reporting and risk treatment plans can then be applied. (Fig. 3) outlines a holistic overview of a chemical substance reporting system.

Based on expert interviews the following data supply chain flow was identified:

- Materials function: define the chemical substance(s); mixture(s) or material(s) to a specification (material / process based).
- Design function: create individual engineering drawing (geometry) data for article(s) with applicable specifications (from the materials function) defining material and process data.
- Purchasing function: responsible for purchasing substance, mixtures and articles from suppliers.

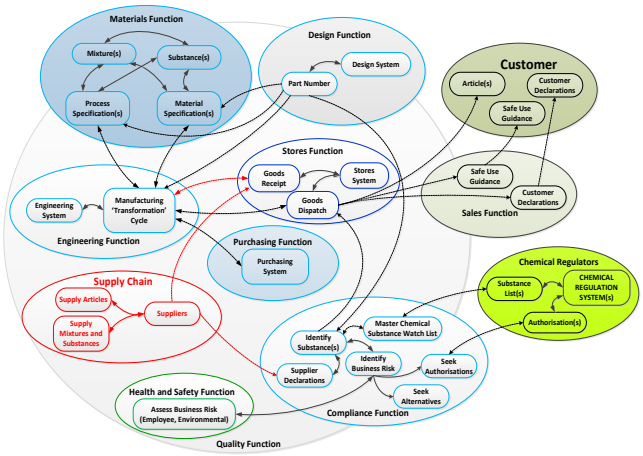

Figure 3. The chemical substance reporting system context model

- Engineering function: responsible for transforming raw materials / semi-components and semi-finished articles into finished articles.
- Stores function: receipt, dispatch articles, together with safe use guidance and customer declarations.
- Compliance function: (1) analyze data from internal systems and data provided by suppliers; (2) data compared to regulatory substance lists to derive obligations (customer declarations and regulatory notifications); (3) risk analysis of any articles at risk from chemical regulations; (4) generate customer material declarations.
- Health and Safety function: ensure safety of employees, users of articles and the environment. This sub-system relies on (1) data provided by materials function relating to substance(s), mixture(s) and material(s); (2) data provided by engineering function relating to substance(s), mixture(s) and material(s) used within manufacturing cycle; (3) all functions providing general safety information.
- Sales function: (1) liaise with customer; (2) distribute any customer declarations including any safe use guidance. This sub-system relies on (3) health and safety function provide any article related safety information; (4) compliance function to provide any material declaration data.
- Quality function: ensure quality is maintained across the organization. This sub-system works across other functional areas to ensure quality procedures are in place.
- Supply chain: supply (1) chemical substance(s); (2) mixture(s); (3) material(s); (4) semi-finished articles and; (5) finished article(s). Suppliers will supply articles to the stores function, providing supplier declarations which detail if any regulated substance(s) are contained within a supplied article(s).
- Chemical regulators: define chemical substances which require compliance reporting, notifications, and potential further restriction.

- Customers: end consumers of articles produced.

Issues arise where variability in data consistency and quality causes incorrect analysis taking place.

E. Infromation Paradox – Typical Checmial Substance Reporting Issues – Examples from AD Industries

Based on expert interviews, common practices identified:

- Design documents: (1) drawings; (2) material / process specifications; (3) machining / assembling / cleaning instructions, etc.
- Contractual documents: (1) supplier agreements; (2) audit data (3) payment terms and conditions; (4) required document(s): (5) statements of conformity; (6) supplier chemical substance declarations; (7) conflict mineral reporting; (8) safe use information; (9) industry reporting standards, etc.

The biggest problem lies in data ambiguity (Fig. 4). Data ambiguity results from (1) poor supplier requirements; (2) poor configuration management of source engineering article definitions; (3) material and process specifications calling out multiple substances, to avoid the cost of issuing new revisions to engineering drawings.

Adopting a one chemical substance or mixture for one specification approach will result in improved configuration management enabling greater substance traceability. The negative aspect will be in the more frequent generation of new engineering drawings.

Maintaining data ambiguity by using many chemical substances to one specification (many to one), incurs cost inefficiencies of having to (1) checking all data from substance(s) to specification; (2) verifying actual substances used to enable determination of declarable and non-declarable chemical substance(s).

F. Chemical Substance Reporting Paradox

- Chemical regulations: state chemical substance(s) that need to be traced and reported above a threshold (ECHA candidate list, 2017; ECHA authorisations list, 2017; ECHA restrictions list, 2017)
- Engineering definitions: state specification(s) which require substance(s), mixture(s) or material(s).
- Supply chain: (1) complex supply chain tiers; (2) spanning multiple nations / regions; (3) cost constraints; (4) competition restrictions; (5) security restrictions (defence); (6) intellectual property issues. The lowest supply chain tier has the most accurate data within the article transformation cycle, as the article is transformed multiple factors (1-6) can constrain the flow of information.

In the context of complex articles, if you ask a supplier to complete a supplier declaration, the response will invariably be 'we produced as per your specification' which then needs additional discussion with a supplier to confirm the precise chemical substances which were used, and why they need to be reported. Thus, envelops a level of angst – additional effort required, which may not have been originally defined in contractual terms / costs.

Category	Sub-Category	Examples of Information	Data Ambiguity Caused By
Contractual Documents	Supplier Agreements	Specific terms – Article supply (batch sizes) / Definition of obligations	(1) Supplier agreements signed for several years in advance; (2) Generic contract clauses for reporting cause confusion; (3) Not defining precise reporting standards; (4) Not stating any reporting requirements.
	Payment Terms	Based on article acceptance	
	Required Documents	Statements of conformity	(1) Data may be spread across multiple sub-systems; (2) Tracing substance(s) across transformation cycle; (3) Understanding declarable data and safe use guidance data to be provided
		Material declarations	
		Conflict mineral reporting	
		Safe use guidance	
		Industry reporting standards	
	Audit Data	Auditing supplier processes and checking required documentation is in place.	(1) Lack of supplier awareness; (2) Poor quality control; (3) Data may be spread across multiple sub-systems.
Design Documents	Engineering Design Documents	Dimensional data.	(1) Identifying substances in articles; (2) Poor document version control management.
	Materials Information	Material specifications	(1) Identifying substances in processes; (2) Poor document version control management.
		Process specifications	

Figure 4. Chemical substance reporting examples of data ambiguity

The chemical substance reporting paradox results in the supply chain reporting struggling to be processed beyond the mid-chain tiers, unless a standardized chemical substance reporting approach is adopted with a standard list of data elements, declarable substances, and template document (XML / Web based) for transmitting requests and receiving data supply data.

G. The Chemical Substance Reporting Framework Model

1) Framework development

A basic requirements analysis model (Fig.5) derived from (Botsford, 2010; Cox and Sweatman, 1999; Deming, 2000). A competency based modelling, known as Knowledge Skill Ability and Other characteristics (KSAO) suggests improving knowledge worker productivity by focusing on and refining the organizational context that influence fast thinking to improve efficiency, effectiveness, and motivation (Campion, 2011; Müller-Frommeyer, 2017; Hawken, Lovins, Lovins, 2013).

The chemical substance reporting framework model presented in the following sub-sections covers:

- Creation of master chemical substance list, to monitor substances, mixtures and materials on hand.
- Creation of data elements to be used within the framework.
- Creation of a supply chain chemical substance reporting questionnaire.
- Map out supply chain data flows.
- Agree supply chain chemical substance reporting.
- Execute supply chain chemical substance reporting requests - push or pull.
- Receive data back.
- Evaluate data received back.
- Evaluate the supply chain chemical substance reporting process and adjust as necessary.

2) Define a master chemical substance list

Review all applicable chemical substance lists (regions where articles are produced and consumed). Create a generic 'Master Chemical Substance List', against which the organization would then take applicable actions (Fig. 6; Fig. 7).

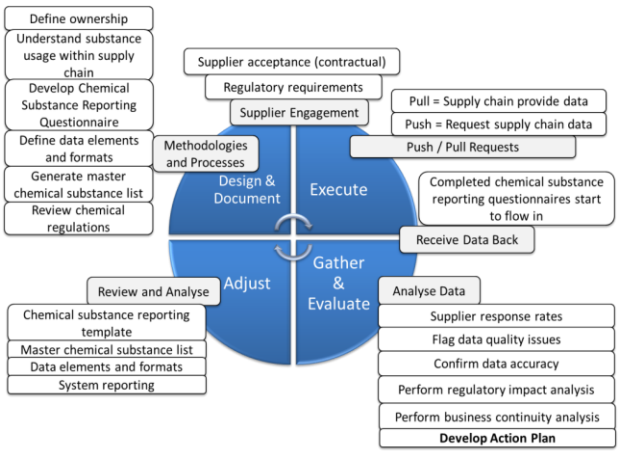

Figure 5. Basic requirements analysis model

3) Define data elements and formats

Review internal data supply chain flows of information, derive a common set of data elements (Fig. 8; Fig. 9; Fig. 10).

Data formats should be simple to use and capable of parsing data. The simplest format to transmit and receive data in is a spreadsheet parsing data in a simple structure. The more advanced formats would be via an XML form.

The master chemical inventory list will act as the reference list against which data from internal supply chain can be queried and analyze any potential business risk(s).

4) Develop a supply chain chemical substance reporting questionnnaire

Define a set of data elements need to be captured as part of a chemical substance reporting supply chain survey (Fig. 11). Existing data exchange standard templates may be used (IPC, 2017; IEC, 2017) may be utilized instead of developing a supply chain questionnaire, the values in (Fig. 11), align to those existing data exchange standards.

5) Understand data flows within a supply chain

Assume articles are defined by specifications which define substances which remain on the finished articles (material specifications) and substances which are used in the process of producing the article (process specification) (Fig. 12).

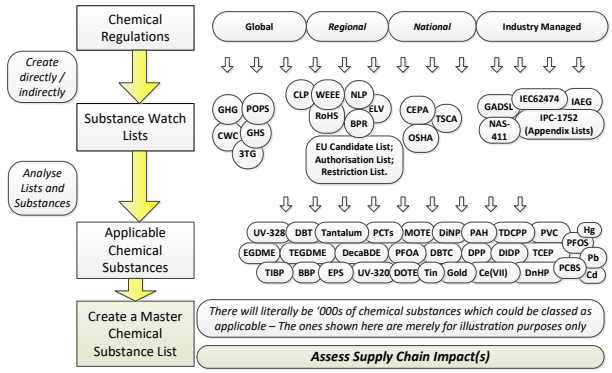

Figure 6. Create a master chemical substance list

Master Chemical Substance List [Declarable Substance List]		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Unique ID Number>	Alphanumeric	Mandatory
<Chemical Substance Name>	Alphanumeric	Mandatory
<CAS Number>	Alphanumeric	Mandatory
<EC Number>	Alphanumeric	Mandatory
<Date of Inclusion>	Date	Mandatory
<Reason for Inclusion>	Alphanumeric	Mandatory
<Status>	Alphanumeric	Mandatory
<Date of Last Update>	Date	Mandatory
<Internal Priority Ranking>	Alphanumeric	Mandatory

Figure 7. Master chemical inventory list (declarable substance list) data elements

Materials Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Specification Name>	Alphanumeric	Mandatory
<Specification Type>	Alphanumeric	Mandatory
<Substance / Mixture ID>	Alphanumeric	Mandatory
<Mixture Name>	Alphanumeric	Mandatory
<Mixture Manufacturer>	Alphanumeric	Mandatory
<Mixture Manufacture Date>	Date	Mandatory
<Mixture Description>	Alphanumeric	Mandatory
<Mixture Use Description>	Alphanumeric	Mandatory
<Substance Name>	Alphanumeric	Mandatory
<Substance Manufacturer>	Alphanumeric	Mandatory
<Safety Data Sheet Name>	Alphanumeric	Mandatory
<Safety Data Sheet Date>	Date	Mandatory
<Substance Description>	Alphanumeric	Mandatory
<Substance Use Description>	Alphanumeric	Mandatory
<CAS Number>	Alphanumeric	Mandatory
<EC Number>	Alphanumeric	Mandatory
<Substance Mass>	Alphanumeric	Mandatory
<Substance Unit of Measure>	Alphanumeric	Mandatory
<Substance Mandatory / Optional>	Alphanumeric	Mandatory
<Substance to Specification Status>	Alphanumeric	*Optional*
<Substance Declarable Status>	Alphanumeric	*Optional*

Design Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Top Level Article Number>	Alphanumeric	Mandatory
<BOM Level>	Numeric	Mandatory
<Assembly Number>	Alphanumeric	Mandatory
<Assembly Description>	Alphanumeric	Mandatory
<Qty>	Numeric	Mandatory
<Geometry Drawing ID>	Alphanumeric	Mandatory
<Specification Name>	Alphanumeric	Mandatory
<BOM Level>	Numeric	Mandatory
<Part Number>	Alphanumeric	Mandatory
<Part Description>	Alphanumeric	Mandatory
<Qty>	Numeric	Mandatory
<Geometry Drawing ID>	Alphanumeric	Mandatory
<Specification Name>	Alphanumeric	Mandatory
<BOM Level>	Numeric	Mandatory
<Component Number>	Alphanumeric	Mandatory
<Component Description>	Alphanumeric	Mandatory
<Qty>	Numeric	Mandatory
<Geometry Drawing ID>	Alphanumeric	Mandatory
<Specification Name>	Alphanumeric	Mandatory
<BOM Level>	Numeric	Mandatory
<Semi-Component Number>	Alphanumeric	Mandatory
<Semi-Component Description>	Alphanumeric	Mandatory
<Qty>	Numeric	Mandatory
<Geometry Drawing ID>	Alphanumeric	Mandatory
<Specification Name>	Alphanumeric	Mandatory
<BOM Level>	Numeric	Mandatory

Figure 8. Material and design functional areas data elements

Engineering Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Top Level Article Number>	Alphanumeric	Mandatory
<Top Level Article Description>	Alphanumeric	Mandatory
<Geometry Drawing>	Alphanumeric	Mandatory
<Machine Program>	Alphanumeric	Mandatory
<Inspection Data>	Alphanumeric	Mandatory
<Assembly Instructions>	Alphanumeric	Mandatory
<Test Data>	Alphanumeric	Mandatory
<Assembly Number>	Alphanumeric	Mandatory
<Assembly Description>	Alphanumeric	Mandatory
<Geometry Drawing>	Alphanumeric	Mandatory
<Machine Program>	Alphanumeric	Mandatory
<Inspection Data>	Alphanumeric	Mandatory
<Assembly Instructions>	Alphanumeric	Mandatory
<Test Data>	Alphanumeric	Mandatory
<Part Number>	Alphanumeric	Mandatory
<Part Description>	Alphanumeric	Mandatory
<Geometry Drawing>	Alphanumeric	Mandatory
<Machine Program>	Alphanumeric	Mandatory
<Inspection Data>	Alphanumeric	Mandatory
<Assembly Instructions>	Alphanumeric	Mandatory
<Test Data>	Alphanumeric	Mandatory
<Component Number>	Alphanumeric	Mandatory
<Component Description>	Alphanumeric	Mandatory
<Geometry Drawing>	Alphanumeric	Mandatory
<Machine Program>	Alphanumeric	Mandatory
<Inspection Data>	Alphanumeric	Mandatory
<Assembly Instructions>	Alphanumeric	Mandatory
<Test Data>	Alphanumeric	Mandatory
<Semi-Component Number>	Alphanumeric	Mandatory
<Semi-Component Description>	Alphanumeric	Mandatory
<Geometry Drawing>	Alphanumeric	Mandatory
<Machine Program>	Alphanumeric	Mandatory
<Inspection Data>	Alphanumeric	Mandatory
<Assembly Instructions>	Alphanumeric	Mandatory
<Test Data>	Alphanumeric	Mandatory

Purchasing Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Material Number>	Alphanumeric	Mandatory
<Material Description>	Alphanumeric	Mandatory
<Supplier ID>	Alphanumeric	Mandatory
<Supplier Name>	Alphanumeric	Mandatory
<Supplier Address>	Alphanumeric	Mandatory
<Supplier Phone>	Numeric	Mandatory
<Supplier Contact Name>	Alphanumeric	Mandatory
<Supplier Contact Phone>	Numeric	Mandatory
<Supplier Contact Email>	Alphanumeric	Mandatory
<Supplier Contact Address>	Alphanumeric	Mandatory
<Supplier Purchase Order No(s)>	Numeric	Mandatory
<Supplier Part Number(s)>	Alphanumeric	Mandatory
<Supplier Contract Batch Size>	Numeric	Mandatory
<Supplier Order Qty>	Numeric	Mandatory
<Supplier Order Date>	Date	Mandatory

Sales Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Material Number>	Alphanumeric	Mandatory
<Material Description>	Alphanumeric	Mandatory
<Customer ID>	Alphanumeric	Mandatory
<Customer Name>	Alphanumeric	Mandatory
<Customer Address>	Alphanumeric	Mandatory
<Customer Phone>	Numeric	Mandatory
<Customer Contact Name>	Alphanumeric	Mandatory
<Customer Contact Phone>	Numeric	Mandatory
<Customer Contact Email>	Alphanumeric	Mandatory
<Customer Purchase Order No(s)>	Numeric	Mandatory
<Customer Part Number(s)>	Alphanumeric	Mandatory
<Customer Contract Batch Size>	Numeric	Mandatory
<Customer Order Qty>	Numeric	Mandatory
<Customer Order Date>	Date	Mandatory

Figure 9. Engineering, purchasing and sales functional areas data elements

Transportation Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Material Number>	Alphanumeric	Mandatory
<Material Description>	Alphanumeric	Mandatory
<Packaging ID>	Alphanumeric	Mandatory
<Packaging Type>	Alphanumeric	Mandatory
<Labelling Data>	Alphanumeric	Mandatory
<Safe Use Guidance>	Alphanumeric	Mandatory
<Dimensional Data>	Alphanumeric	Mandatory
<Customer / Supplier Name>	Numeric	Mandatory
<Customer /Supplier Contact Email>	Alphanumeric	Mandatory
<Dispatch Address>	Alphanumeric	Mandatory
<Dispatch Method>	Alphanumeric	Mandatory
<Dispatch Reference>	Alphanumeric	Mandatory
<Dispatch Date>	Date	Mandatory

Health and Safety Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Material Reference ID>	Alphanumeric	Mandatory
<Mixture Name>	Alphanumeric	*Optional*
<Mixture Description>	Alphanumeric	*Optional*
<Mixture Risk Analysis>	Alphanumeric	*Optional*
<Mixture Risk Actions>	Alphanumeric	*Optional*
<Mixture Review Date>	Date	*Optional*
<Substance Name>	Alphanumeric	Mandatory
<Substance Description>	Alphanumeric	Mandatory
<Substance Risk Analysis>	Alphanumeric	Mandatory
<Substance Risk Actions>	Alphanumeric	Mandatory
<Substance Review Date>	Date	Mandatory

Quality Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Quality Procedure ID>	Alphanumeric	Mandatory
<Applicable Function Name>	Alphanumeric	*Optional*
<Quality Procedure Name>	Alphanumeric	Mandatory
<Quality Procedure Data>	Alphanumeric	Mandatory
<Quality Procedure Review Date>	Date	Mandatory

Compliance Function		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Chemical Substance Reporting Questionnaire ID>	Alphanumeric	Mandatory
<Reporting Questionnaire Type>	Supplier / Customer / Request for Additional Data	Mandatory
<Reporting Questionnaire Supplier Transmitted To>	Alphanumeric	Mandatory
<Reporting Questionnaire Supplier Initial Request Date>	Date	Mandatory
<Reporting Questionnaire Status>	Sent / Received	Mandatory
<Customer Declaration ID>	Alphanumeric	Mandatory
<Customer Declaration Transmitted to>	Alphanumeric	Mandatory
<Customer Declaration Transmitted Date>	Date	Mandatory
<Customer Declaration List of Affected Articles>	Alphanumeric	Mandatory
<Customer Declaration List of Substances on Articles>	Alphanumeric	Mandatory
<Customer Declaration Statement>	Alphanumeric	Mandatory
<Positive Declaration ID>	Alphanumeric	Mandatory
<Supplier Positive Declaration Transmitted to>	Alphanumeric	Mandatory
<Supplier Positive Declaration Transmitted Date>	Date	Mandatory
<Supplier Positive Declaration List of Affected Articles>	Alphanumeric	Mandatory
<Supplier Positive Declaration List of Substances on Articles>	Alphanumeric	Mandatory
<Sunset Date on Substances on / in Article(s)>	Alphanumeric	Mandatory
<Request Supplier Region Where Substance Used >	Alphanumeric	Mandatory
<Request Awareness of Sunset Date >	Yes / No	Mandatory
<Request Supplier Replacement Strategy >	Alphanumeric	Mandatory
<List of Exemptions Applied >	Alphanumeric	Mandatory
<List of Exemptions Received >	Alphanumeric	Mandatory
<List of Exemption Substances >	Alphanumeric	Mandatory
<List of Authorisations Applied >	Alphanumeric	Mandatory
<List of Authorisations Received >	Alphanumeric	Mandatory
<List of Authorisations Substances >	Alphanumeric	Mandatory

Figure 10. Transportation, health and safety, quality and compliance functional areas data elements

Requestor Contact Details		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Requestor Company Name>	Alphanumeric	Mandatory
<Requestor Individual Name>	Alphanumeric	Mandatory
<Requestor Address>	Alphanumeric	Mandatory
<Requestor Phone Number>	Numeric	*Optional*
<Requestor Email Address>	Alphanumeric	Mandatory
<Requestor Form ID>	Alphanumeric	Mandatory
<Requested Date>	Date	Mandatory
Respond By Date	Date	*Optional*
Requestor Comments	Alphanumeric	*Optional*

Terms and Definitions (Legal Statements – for example information supplied on a best endeavours basis)		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Terms and Conditions>	Alphanumeric	Mandatory

Supplier Contact Details		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Supplier Company Name>	Alphanumeric	Mandatory
<Supplier Name>	Alphanumeric	Mandatory
<Supplier Company ID>	Alphanumeric	Mandatory
<Supplier Individual Name>	Alphanumeric	Mandatory
<Supplier Address>	Alphanumeric	Mandatory
<Supplier Phone Number>	Numeric	*Optional*
<Supplier Email Address>	Alphanumeric	Mandatory
<Supplier Response Date>	Date	Mandatory
<Declarable Substance List (DSL) Name>	Alphanumeric	Mandatory
<DSL Version Name>	Alphanumeric	Mandatory
<DSL Version Date>	Date	Mandatory
<Supplier Comments>	Alphanumeric	Mandatory

Article Declaration Data (for example Part / Assembly / Product)		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Requestor Article Number>	Alphanumeric	Mandatory
<Requestor Article Name>	Alphanumeric	Mandatory
<Requestor Article Version>	Alphanumeric	Mandatory

Article Declaration Data (for example Part / Assembly / Product)		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Supplier Article BOM Level>	Alphanumeric	*Optional*
<Supplier Article Number>	Alphanumeric	Mandatory
<Supplier Article Name>	Alphanumeric	Mandatory
<Supplier Article Version>	Alphanumeric	Mandatory
<Country of Manufacture>	Alphanumeric	Mandatory
<Number of Instances>	Numeric	Mandatory
<Supplier Article Weight>	Alphanumeric	Mandatory
<Supplier Article UoM>	Alphanumeric	Mandatory
<Specification / Standard Used>	Alphanumeric	*Optional*
<Material Name>	Alphanumeric	*Optional*
<Material Manufacturer>	Alphanumeric	*Optional*
<Mixture Use Description>	Alphanumeric	*Optional*
<Mixture UoM>	Alphanumeric	*Optional*
<Mixture Mass>	Alphanumeric	*Optional*
<Mixture – Finished Product or Just for Process of Manufacture>	True / False	*Optional*
<Chemical Substance Name>	Alphanumeric	*Optional*
<Substance CAS Number>	Alphanumeric	*Optional*
<Substance EC Number>	Alphanumeric	*Optional*
<DSL ID Number>	Alphanumeric	*Optional*
<Substance Use Description>	Alphanumeric	*Optional*
<Substance Mass>	Alphanumeric	*Optional*
<Substance UoM>	Alphanumeric	*Optional*
<Substance – Finished Product or Just for Process of Manufacture>	True / False	*Optional*
<Substance Is Article?>	True / False	*Optional*
<Substance Is Homogenous?>	True / False	*Optional*
<Substance Affected by RoHS?>	True / False	*Optional*
<RoHS Exemption Number (if applicable)>	True / False	*Optional*

Supplier Sign-Off Information		
Data Element Name	**Data Element Type**	**Mandatory / Optional**
<Attachment>	[File Attachment]	*Optional*
<Authoriser Name>	Alphanumeric	Mandatory
<Declaration Type>	Full / Partial / Incomplete	Mandatory
<Authoriser Comments>	Alphanumeric	Mandatory
<Authorisation Date>	Date	Mandatory

Figure 11. Chemical substance reporting questionnaire data elements

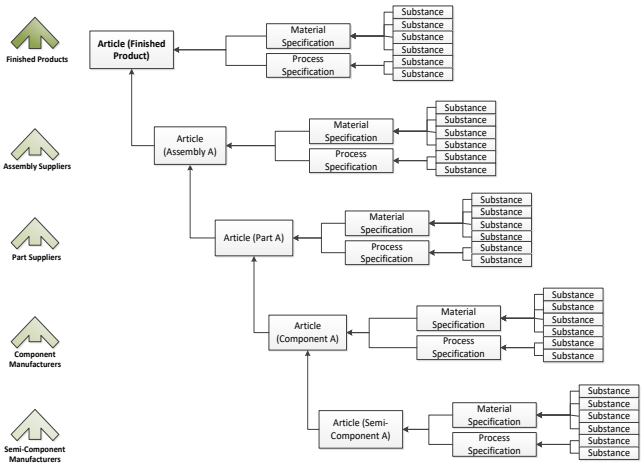

Figure 12. Substance usage within the article transformation process

Information flows from the lowest tiers (raw chemical suppliers / refiners / formulators / mixers) are the most detailed as it generally pertains to the Materials Safety Data Sheet and Safety Data Sheet data, in which chemical substances/ exposure / handling / labelling data is presented to users.

Define ownership:

- Which department / function / team will be responsible for the transmission and receipt of the data from the supply chain?
- What training will be given to the supply chain?
- How will the training be communicated?
- How will the data be receipted back, which data formats are acceptable?
- How will end user queries be handled?

6) Agree supply chain chemical substance reporting

- Establish an early supplier engagement process.
- Ensure suppliers have contract coverage which states the need for chemical substance reporting as part of a 'business as usual' process.
- Ensure training developed for the supply chain informs them about their legal obligations to report chemical substance presence, above designated threshold levels, regardless of a part being defined by your organization or the external supplier.
- Establish supply awareness of any chemical substance reporting templates as soon as possible to identify issues prior (via a simple pilot) to being rolled out to your entire supply chain.

7) Execute supply chain chemical supporting reporting requests – push or pull?

- A push chemical substance reporting system exists where the lowest supply chain tiers flows information to downstream users within a supply chain (Fig. 13). Push chemical substance reporting systems work best in industries where the articles are regulated and highly defined.

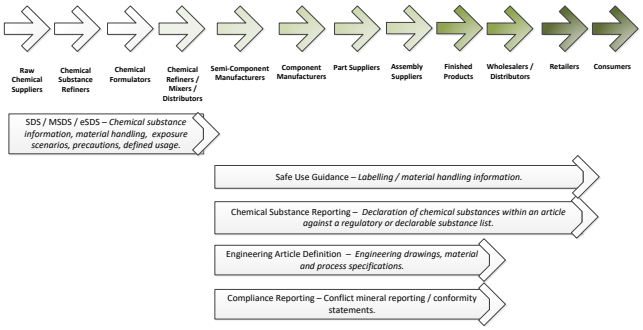

Figure 13. Article transformation cycle: push chemical substance reporting system

- Complex articles need to be considered as those with high potential data ambiguity. They will require a pull type chemical reporting system, where the highest tiers are initiating the chemical substance reporting information requests to the lowest tiers (upstream) who will then flow the information back (downstream) (Takhar and Liyanage, 2017)

8) Receive data back

- Chemical substance reporting questionnaires start to flow back, ensure the data is receipted and stored in a defined location for processing.
- From a defined location, the data should be collected (automated or manual) and then ingested into a target system. The target system will then process the data.
- Processed files should then be moved to a processed folder to be used in the event of a system failure.

9) Evaluate data received back

- Supplier response rates: record as a set of metrics the dates, names of suppliers who have (pull requests) transmitted completed chemical reporting questionnaires back to the organization.
- Flag data quality issues: either check all the responses or perform a spot check analysis on a sample set. Flag issues back to respondents where issues have arisen.
- Perform regulatory impact analysis: run reporting which compares data and highlights chemical

substances which potentially require (1) threshold declarations to customers / regulators; (2) require authorizations for continued usage; (3) have been flagged as restricted for specific use condition.

- Perform business continuity analysis: substances flagged as requiring action (because of performing regulatory impact analysis), identify where these substances are used within the organization or across the supply chain.
- Develop an action plan: plan the actions which need to be undertaken such as declarations; authorizations; looking for alternative substances; performing last time purchases.

10) Evaluate the supply chain chemical substance reporting process and adjust as necessary

- Chemical substance reporting template: use feedback from your supply chain and make any necessary adjustments.
- Master chemical substance list: this will require regular updates as more and more chemicals become regulated, adjust the list regularly.
- Data elements and formats: use feedback from your supply chain and adjust as required.
- System reporting: adjust reporting as required.
- Additional declarations: where a supplier has flagged the use of a substance of concern, an additional declaration may be required as to understand actions supplier strategy regarding looking for alternative substances.

H. Implementing the Chemical Substance Reporting Framework Model

1) Business function support of the framework model

The chemical substance reporting data model (Fig. 14), the design of this model should allow for analysis and reporting against REACH, RoHS and other regulatory chemical substance reporting.

The data model will also additionally feed into EU Classification, Labelling and Packaging (CLP) (EU CLP, 2017), EU Biocidal Properties Reporting (BPR) (EU BPR, 2012; EU BPR, 2014) and EU Conflict Mineral Reporting (CMR) (EU CMR, 2017) reporting. The outputs could additionally be used to feed into Life Cycle Assessment (LCA) as a secondary data set.

2) Where could the chemical substance data be stored?

The core aim of the chemical substance reporting data model depicts the data elements needed to perform chemical substance reporting as well as the required data elements from an organizations data supply chain.

The chemical substance reporting data model can be implemented in a few different IT systems and platforms (Table I).

The data model can be applied as either a (1) stand-alone system or; (2) applicable functional data elements added to sub-systems, with data exported to a central reporting solution or; (3) a central reporting solution queries the functional sub-systems.

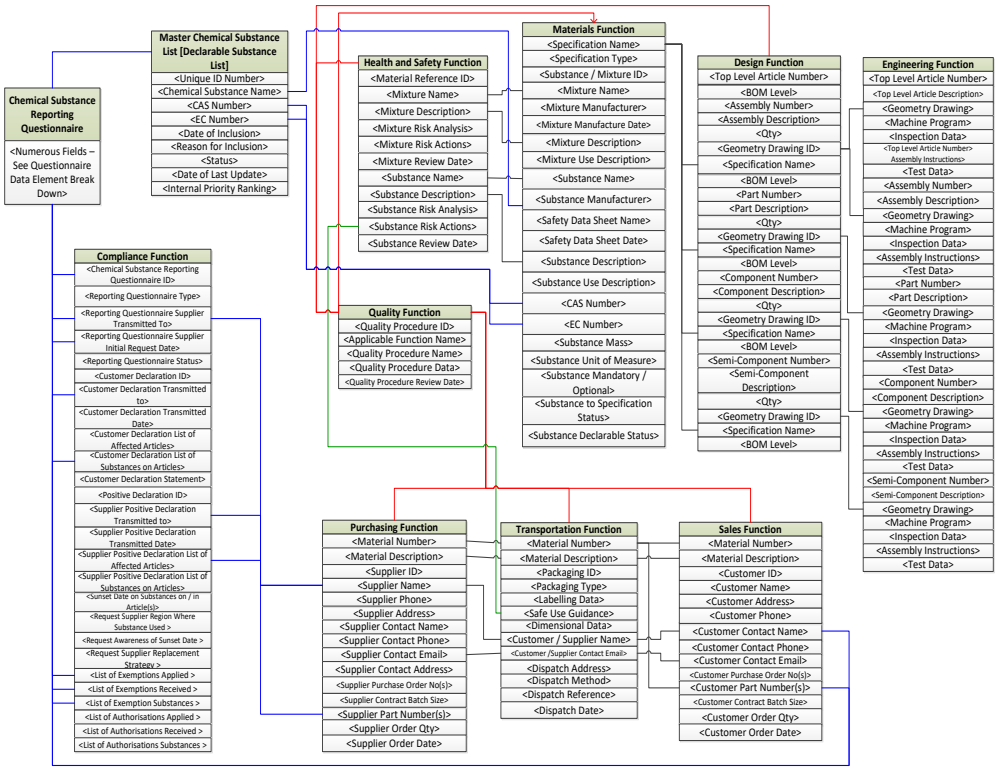

Figure 14. Chemical substance reporting data model

TABLE I. FUNCTIONS, SYSTEMS AND RELACTED IT SYSTEM TYPES

Functional area	Safety Data Sheet System	Material Specification System	Compliance Reporting (REACH / CMR / CLP / PBR / ELV / Supply Chain Engagement)	CAD Drawing System	PDM / PLM Systems	ERP System	Manufacturing Execution System (Machining / Inspection)	Technical Publications
Chemical Substance Reporting Questionnaire			X					
Compliance Function			X		X			
Master Chemical Substance list	X	X	X					
Health and Safety Function	X		X				X	
Quality Function	X	X	X		X	X	X	X
Materials Function	X	X	X					
Design Function			X	X	X			
Engineering Function			X	X	X		X	X
Purchasing Function			X		X	X		
Transportation Function			X			X		
Sales Function						X		X

3) Examples of checmical substance reporting

- Initial business impact: system shall can identify which substances using the master chemical substance list.
- Extended impacts: (1) report against the article / higher level assembly article sales data to understand the gauge the potential sales impact; (2) consider the burden of an article being removed from the supply chain; (3) assess chemical substance import levels (based on substance name, supplier name and locational details).
- Assess if any substance import notifications are to be performed.
- Customer declarations: (1) inform customers of a substance presence above a threshold (2) supply at a name of the substance; (3) supply any safe use guidance as required.

4) Data cleansing

Dependent on the levels data ambiguity which exists within the data supply chain, data cleansing may be required, to ensure rich data, data cleansing will include:

- Update source systems / chemical substance reporting system: with a known specification to substance relationship identified, additional processing could be initialized to request confirmation of data from the materials function as to data cleanliness / accuracy. Optional data elements have been added to the materials function section to enable this via the data elements labelled (1) 'substance to specification status' (to denote current / legacy substance) and the (2) 'substance declarable status' (to denote no longer used / removed / trace only / substance is declarable)
- Internal data supply chains: If the sub-systems are data silos which cannot readily exchange data, then investigate the use of exporting data, performing data manipulation and then importing data into the main chemical substance reporting system.

IV. CONCLUSIONS

Chemical regulations will continue to regulate more and more chemical substances. Industry needs to develop chemical reporting systems to record internal and external supply chain usage of chemical substances, to enable appropriate reporting to chemical regulators, employees and end consumers.

Without a chemical reporting system, there is a real potential for business continuity risks to arise from: (1) not clearly understanding hazardous substances being consumed and taking the appropriate safety measures; (2) loss of access to a market if no safety data can be provided; (3) potential financial penalties for not identifying regulated chemical substance(s) in a timely manner, and notifying a regulator; (4) supply chain disruption if raw material(s) cannot be sourced as they contain restricted substance(s); (5) potential product failures if a supplier has changed a material / formulation, which affects the performance of a product, which has not been recorded correctly within existing systems; (6) missing out on the potential benefits of sustainability (Woinaroschy, 2016) and green chemistry (Charpentier, 2016), recycling and reusing critical materials with limited supply back into the supply chain.

The intent of the framework is to provide a footprint data model, which could be implemented within any organization. To implement this data model, an organization can choose:

a) Extend existing sub-systems to collate additional data elements which can then feed into a master chemical substance reporting system;
b) Where used analysis: with the substance to specification, and specification to article definitions in place, the system should be able to run reports identifying the use of substances, specifications, articles. Note this data may have been stored in a 'data silo' mentality across many internal sub-systems.

The current framework has examined the need to identify a substance(s) on an article, as defined by current chemical regulations, future extensions to this framework include

material flow analysis (Zschieschang, 2014) and decision based modelling (Dumas, Schmidt, Alexandera, 2016)

ACKNOWLEDGMENT

Many thanks to the organizations that participated in the expert interviews discussions.

REFERENCES

[1] Dias, L.S., and Ierapetritou, M.G. (2017) From process control to supply chain management: An overview of integrated decision making strategies, *Computers and Chemical Engineering*, **106**, 826-835.

[2] Porter, M.E (1980) *Competitive strategy: techniques for analyzing industries and competitors*, New York: The Free Press, 3-75.

[3] *Regulation of chemicals wiki* (2017) last modified 18 October 2017 [Online]. Available from: https://en.wikipedia.org/wiki/Regulation_of_chemicals, [Accessed 20 September 2017].

[4] IMDS (2017) *Global automotive declarable substance list - background information* [Online]. Available from: https://public.mdsystem.com/en/web/imds-public-pages/gadsl, [Accessed 14 July 2017].

[5] IPC (2017) *IPC-1752* [Online]. Available from: http://www.ipc.org/ContentPage.aspx?pageid=Materials-Declaration#1752a, [Accessed 3 August 2017].

[6] IEC (2017) *IEC-62474* [Online]. Available from: http://std.iec.ch/iec62474, [Accessed 3 August 2017].

[7] IAEG (2017) *IAEG AD-DSL* [Online]. Available from: http://www.iaeg.com/workgroups/wg1/addsl/, [Accessed 3 August 2017].

[8] Botsford, K. (2010) Preparing for product environmental compliance a method for the madness, *Product Compliance Engineering (ISPCE), 2010 IEEE Symposium on*, Boston, MA, USA 2010.

[9] Cox, D., and Sweatman, A. (1999) Management of restricted substances in consumer products, IEEE Xplore Conference: Environmentally conscious design and inverse manufacturing, 1999. Proceedings. *EcoDesign '99: First International Symposium on*, Tokyo, Japan, 1999.

[10] Deming, W.E (2000) *Out of the crisis*, 2nd edition, Massachusetts: MIT Center for Advanced Engineering Study, Massachusetts.

[11] Campion, M.A. et al (2011) *Doing competencies well: best practices In competency modeling*, Personnel Psychology, **64** (1), 225-262.

[12] Müller-Frommeyer, L.C. et al (2017) *Introducing competency models as a tool for holistic competency development in learning factories: Challenges, example and future application, Procedia Manufacturing*, **9**, 307-314.

[13] Hawken, P., Lovins, A.B., Lovins, L.H (2013) *Natural capitalism: The next industrial revolution*, New York: Routledge.

[14] Ashby, M.F. (2009) *Materials and the Environment Eco-Informed Material Choice*, Oxford: Butterworth-Heinemann imprint of Elsevier Inc., 85-99.

[15] Molander, L. et al. (2012) Are chemicals in articles an obstacle for reaching environmental goals? — Missing links in EU chemical management, *Science of The Total Environment*, **435–436**, 280-289.

[16] European Commission (2002) *EU RoHS Directive 2002/95/EC*, Luxembourg: Office for Official Publications of the European Commission.

[17] European Commission (2011) *EU RoHS recast Directive 2011/65/EU*, Luxembourg: Office for Official Publications of the European Commission.

[18] European Commission (2006) *EC REACH Regulation EC 1907/2006* Luxembourg: Office for Official Publications of the European Commission

[19] Skinner, W. (1978) *Manufacturing in the corporate strategy*, New York: Wiley, 25-124.

[20] ECHA (2017) *ECHA candidate list* [Online]. Available from: https://echa.europa.eu/candidate-list-table, [Accessed 15 November 2017].

[21] ECHA (2017) *ECHA authorisations list* [Online]. Available from: https://echa.europa.eu/authorisation-list, [Accessed 15 November 2017].

[22] ECHA (2017) *ECHA restriction list* [Online]. Available from: https://echa.europa.eu/substances-restricted-under-reach, [Accessed 15 November 2017].

[23] Takhar, S. and Liyanage, K. (2017) Top down or Bottom up? - Supply chain engagement for material compliance reporting, *Advances in Transdisciplinary Engineering*, **6**, 77-83.

[24] EU (2017) *CLP* [Online]. Available from: https://echa.europa.eu/regulations/clp/understanding-clp, [Accessed 20 November 2017].

[25] EU (2017) *EU BPR Regulation 528/2012*, Luxembourg: Office for Official Publications of the European Commission.

[26] EU (2014) *EU BPR Regulation 1062/2014*, Luxembourg: Office for Official Publications of the European Commission.

[27] EU (2017) *EU Conflict Minerals Regulation*, Luxembourg: Office for Official Publications of the European Commission.

[28] Selin, H. (2011) Global governance and regional centers: multilevel management of hazardous chemicals and wastes, *Procedia - Social and Behavioral Sciences*, **14**, 40-43.

[29] Molander, L., and Rudén, C. (2012) Narrow-and-sharp or broad-and-blunt – Regulations of hazardous chemicals in consumer products in the European Union, *Regulatory Toxicology and Pharmacology*, **62** (3), 523-531.

[30] Woinaroschy, A. (2016) A paradigm-based evolution of chemical engineering, *Chinese Journal of Chemical Engineering*, **24** (5), 553-557.

[31] Charpentier, J.C (2016) What Kind of Modern 'Green' Chemical Engineering is Required for the Design of the 'Factory of Future'?, *Procedia Engineering*, **138**, 445-458,

[32] Sivaprakash, P., Karthikeyan, L.M, and Joseph, S. (2014) A Study on Handling of Hazardous Chemicals in Engineering Industries, *APCBEE Procedia*, **9**, 187-191.

[33] Zschieschang, E. et al. (2014), Resource Efficiency-oriented Optimization of Material Flow Networks in Chemical Process Engineering, *Procedia CIRP*, **15**, 373-378.

[34] Dumas, D., Schmidt, L.C., and Alexandera, P.A (2016) Predicting creative problem solving in engineering design, *Thinking Skills and Creativity*, **21**, 50-66.

[35] European Commission (1967) *Dangerous Substances Directive 67/548/EEC*, Luxembourg: Office for Official Publications of the European Commission.